Exercise Sheet 6 due 27 November 2014

1. *operators and expectation values*
   i. If the eigenenergies of the Hamiltonian $\hat{H}$ are E_n and the eigenfunctions are φ_n, what are the eigenvalues and eigenfunctions of the operator $\hat{H}^2 - \hat{H}$?

   ii. Consider the equal linear superposition $|\varphi\rangle = (|\varphi_1\rangle + |\varphi_2\rangle)/\sqrt{2}$ of the two lowest eigenstates of an infinitely deep potential well. What are the expectation values of

   (a) the energy ($\int \overline{\varphi(x)}\, \hat{H}\, \varphi(x)\, dx$),
   (b) the momentum ($\int \overline{\varphi(x)}\, \hat{p}\, \varphi(x)\, dx$), and
   (c) the position ($\int \overline{\varphi(x)}\, \varphi(x)\, dx$)?

2. *Hermitian and Unitary operators*
   i. Show that the momentum operator $\hat{p} = -i\hbar\vec{\nabla}$ is Hermitian. For simplicity, you may perform this proof for a one-dimensional system. (Why?)

   Hint: Consider $\int \overline{\varphi_n(x)} \hat{p}_x\, \varphi_m(x)\, dx$, where the $\varphi_n(x)$ are a complete orthonormal set and integrate by parts. Note that the $\varphi_n(x)$ must vanish at infinity, as otherwise they could not be normalized.

   ii. Is the second derivative $\frac{d^2}{dx^2}$ Hermitian?

   iii. Is a Hamiltonian with a real potential Hermitian?

   iv. Show that $\exp(i\hat{M})$ is unitary if $\hat{M}$ is Hermitian.

   v. Show that the exponential $\exp(i\hat{p}_x L/\hbar)$ of the momentum $\hat{p}_x = -i\hbar \frac{d}{dx}$ is a translation operator, i.e. $\exp(i\hat{p}_x L/\hbar)\, \varphi(x) = \varphi(x + L)$.
   Hint: Expand the exponential in a power-series.

3. *Time-dependence of expectation values*

Consider an operator $\hat{A}$ that does not depend on time (i.e., $\partial\hat{A}/\partial t = 0$) and that commutes with the Hamiltonian $\hat{H}$. Show that the expectation value of this operator, for any state $|\Psi(t, \vec{r})\rangle$, does not depend on time, i.e., $\partial\langle\hat{A}\rangle/\partial t = 0$.

4. *Spectral representation*
   i. A Hermitian operator $\hat{A}$ has a complete orthonormal set of eigenfunctions $|\varphi_n\rangle$ with associated eigenvalues α_n. Show that we can always write $\hat{A} = \sum \alpha_n |\varphi_n\rangle\langle\varphi_n|$. This expansion in its eigenfunctions is particularly useful for evaluating functions of $\hat{A}$. To see this, find a simple expression for the inverse, $\hat{A}^{-1}$. Next, find the spectral representation of $f(\hat{A})$ for some function f.

   ii. Show that the trace of a Hermitian operator $\hat{A}$, $\mathrm{Tr}(\hat{A})$, is always equal to the sum of the eigenvalues.